

Tetrahydrophthalic anhydride
85-43-8 | DTXSID3026516

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 6.68e-03 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.65e-01

Confidence level: 3.12e-01

Nearest Neighbors from the Training Set

Image not found

Acenaphthene

Measured: 5.17e-04

Predicted: 1.84e-03

Image not found

Dimethyl methylphosphonate

Measured: 5.25e-02

Predicted: 4.75e-01

Image not found

Acetic acid, trichloro-, ethyl ester

Measured: 1.25e-03

Predicted: 3.75

Image not found

Carbazole

Measured: 2.00e-03

Predicted: 1.90e-05